



Geostatistical Temporal-Spatial Algorithm (GTS)

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LTMO

Introduction

- First seeds of GTS planted in 1997
 - AFCEE interested in new optimization strategy
 - Phil Hunter, AFCEE project lead
 - Decision-logic trees, Fortran routines
- Development of GTS software begun in 2004
 - Current 1.0 prototype only covers 2D scenarios
 - Future versions to handle 2.5D, 3D analyses

What is GTS?

- Geostatistical & statistical LTM optimization program
 - Data-driven, empirical
 - Identifies statistical redundancies
 - Separate temporal, spatial optimization modules
- More details located at AFCEE website
 - <http://www.afcee.brooks.af.mil/products/rpo/>

GTS Version 1.0

- Windows-based freeware
 - Will be available from AFCEE website
 - Detailed decision-logic diagrams also available
- Stitches together components in 3 areas:
 - Exploratory analysis
 - Temporal optimization
 - Spatial optimization

GTS Underpinnings

- Focus on statistical redundancy
 - Assumptions
 - Semi-stable LTM program in place
 - Monitoring data used to make maps, estimate trends
 - Too much data might exist
 - Institutional willingness to 'pare down' sampling program if loss of information minimized
 - Redundancy identified when:
 - Maps, trends accurately estimated with less data

GTS Flowpath

- Pre-GTS Data Preparation
- Exploratory analysis
- Temporal Optimization
- Spatial Optimization

Minimal Requirements

- 20-30 distinct well locations
- Well-defined site boundaries
- 8-10 samples per well for iterative thinning
 - OK to have less with temporal variogram
 - Seasonality not a problem

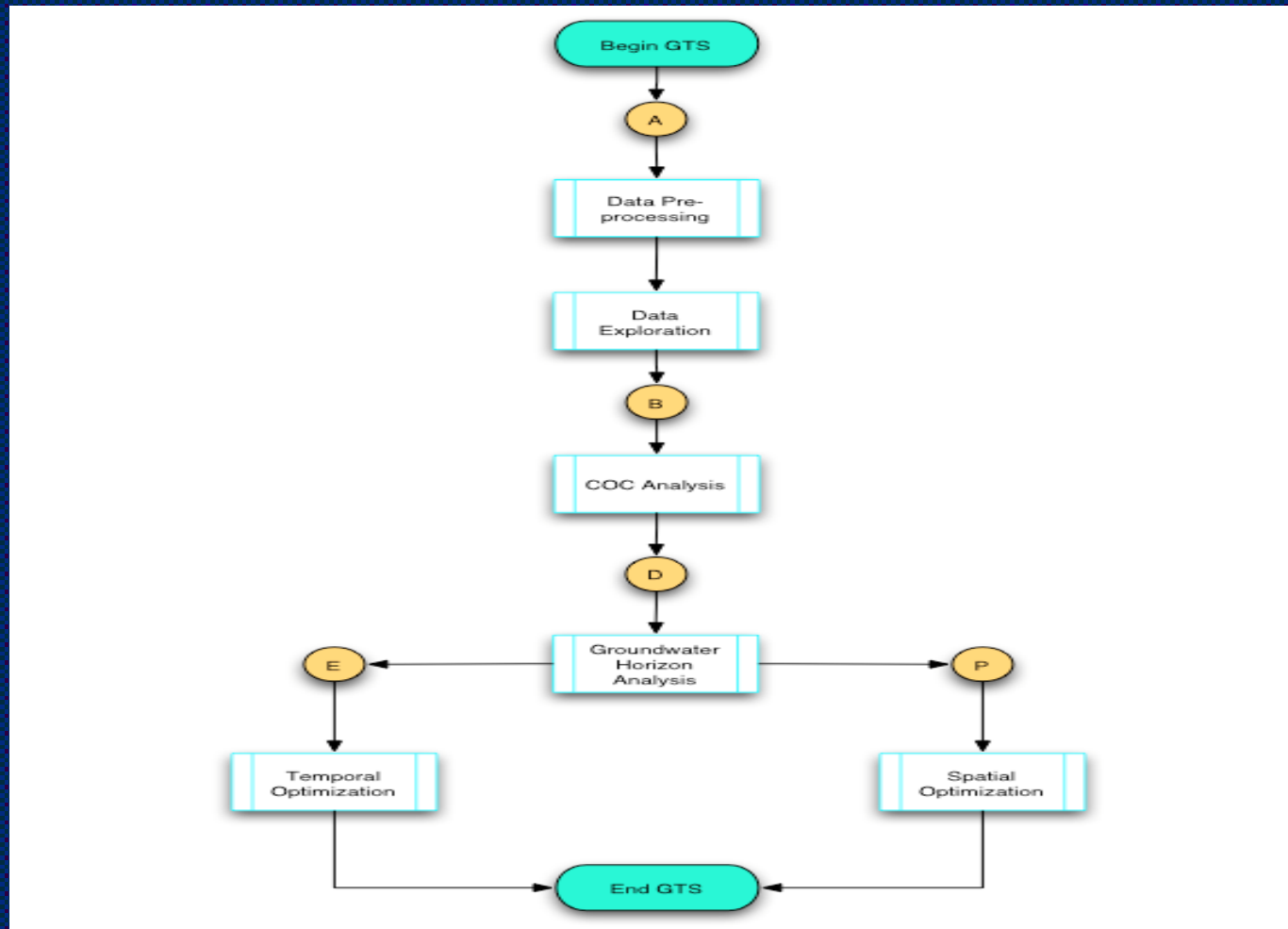
Before Using GTS

- Data gathering, processing
 - Building electronic files
 - Historical data
 - Normalizing formats, units
 - Eliminating duplicates; reconciling discrepancies
- Preparing data for analysis
 - Narrow down to potentially useful COCs
 - Site boundary file
 - Identifying each well screen in 3-dimensions
 - Easting (X), Northing (Y), Depth (Z)
 - Surface elevation
 - Aquifer zones

Before GTS (cont.)

- Handling non-detects
 - Every sample record must have qualifier flag
 - PARVQ: =, TR, ND
 - Set PARVAL = RL/2 or MDL/2 if ND
 - Set PARVAL to measured/estimated value otherwise
- MCLs, regulatory limits
 - Each COC should have a limit
 - Can use secondary MCLs, other limits

GTS Overview



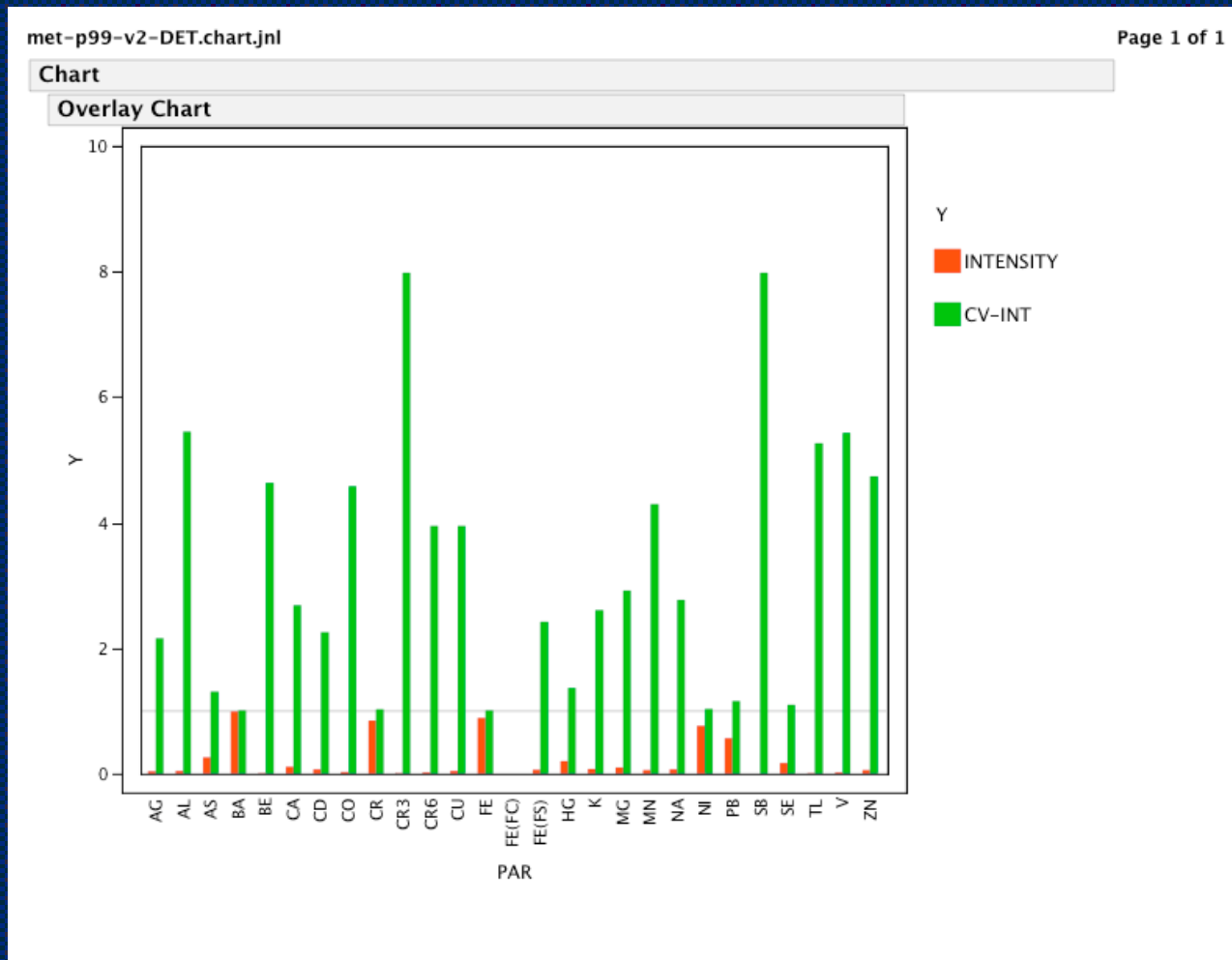
Exploratory Analysis

- Examine site documentation
 - Site maps
 - GW reports
 - Post-plots of well network
- COC analysis
 - Goal: narrow analysis to 2-3 promising parameters
 - Important factors:
 - Known and/or politically sensitive contaminants
 - Frequent, widespread occurrence
 - High spatial intensity & spread

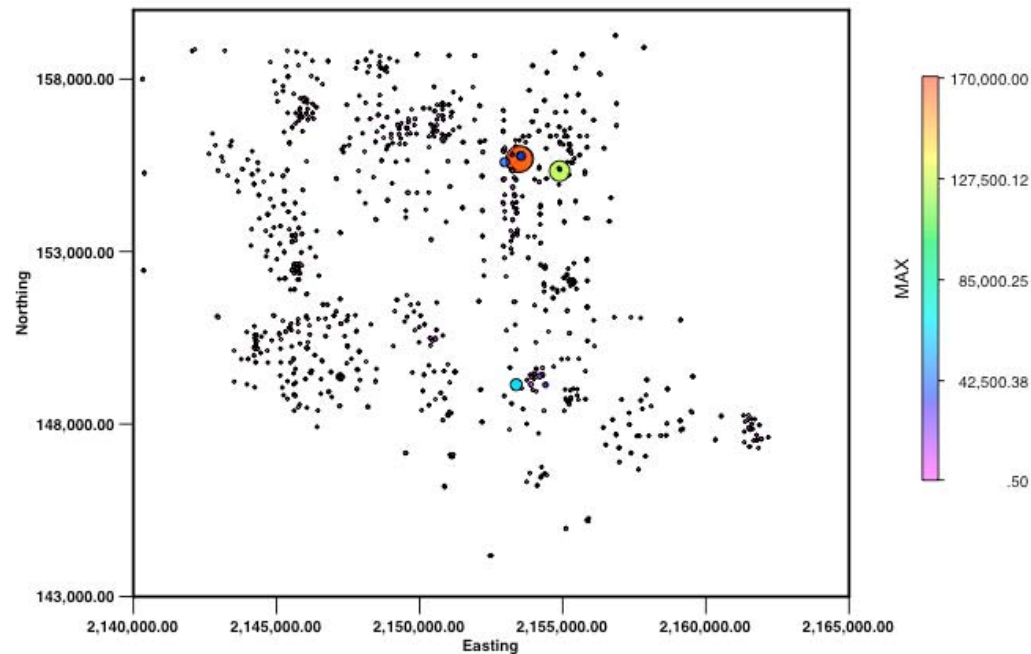
COC Analysis

- Summary statistics
 - Detection rates
 - MCL exceedances
- Spatial intensity, spread
 - Screening tool
 - Compare baseline configuration vs. detected wells, “above-limit” wells
- Concentration maps
 - Well medians, maximums
 - Decile plots

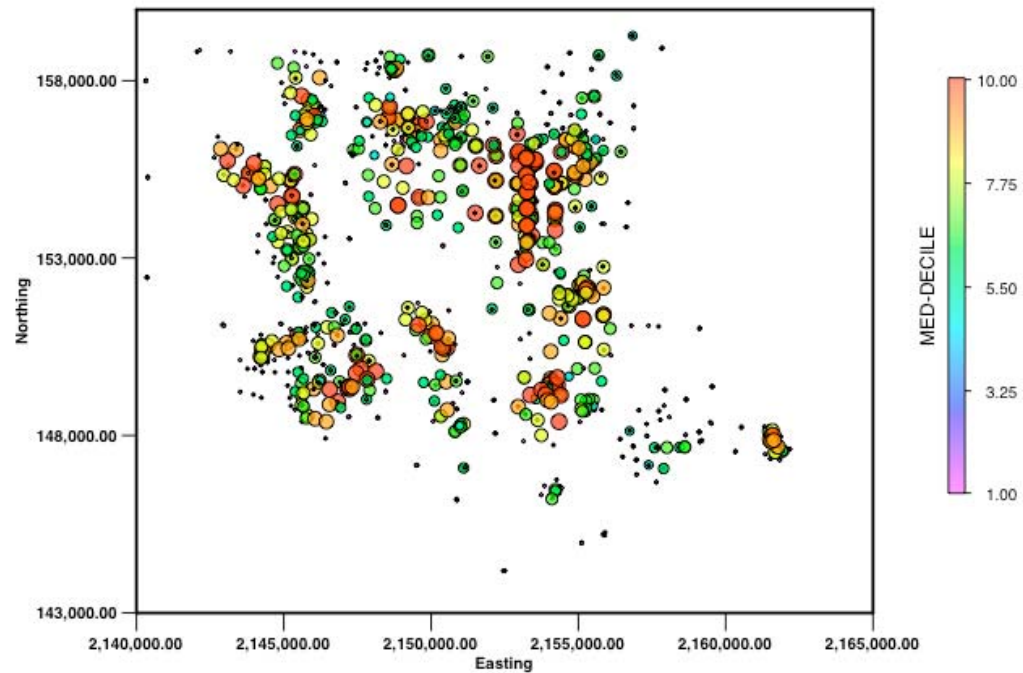
Tinker AFB: Metals Intensity



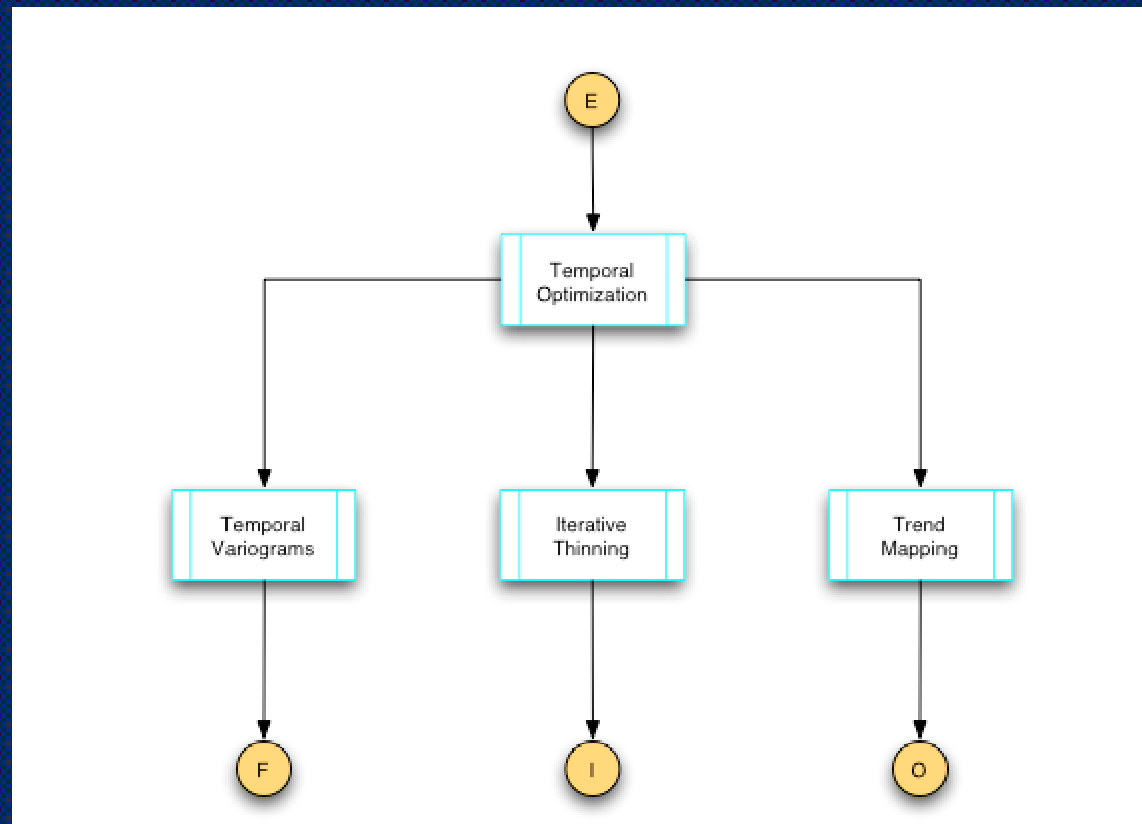
Tinker AFB: Max Post Plot



Tinker AFB: Median Deciles



Temporal Analysis



Guided Example

- Hanford nuclear facility (DOE)
 - Site 300-FF-5
 - 38 wells located near Columbia river
 - Elevated uranium concentrations in ground water

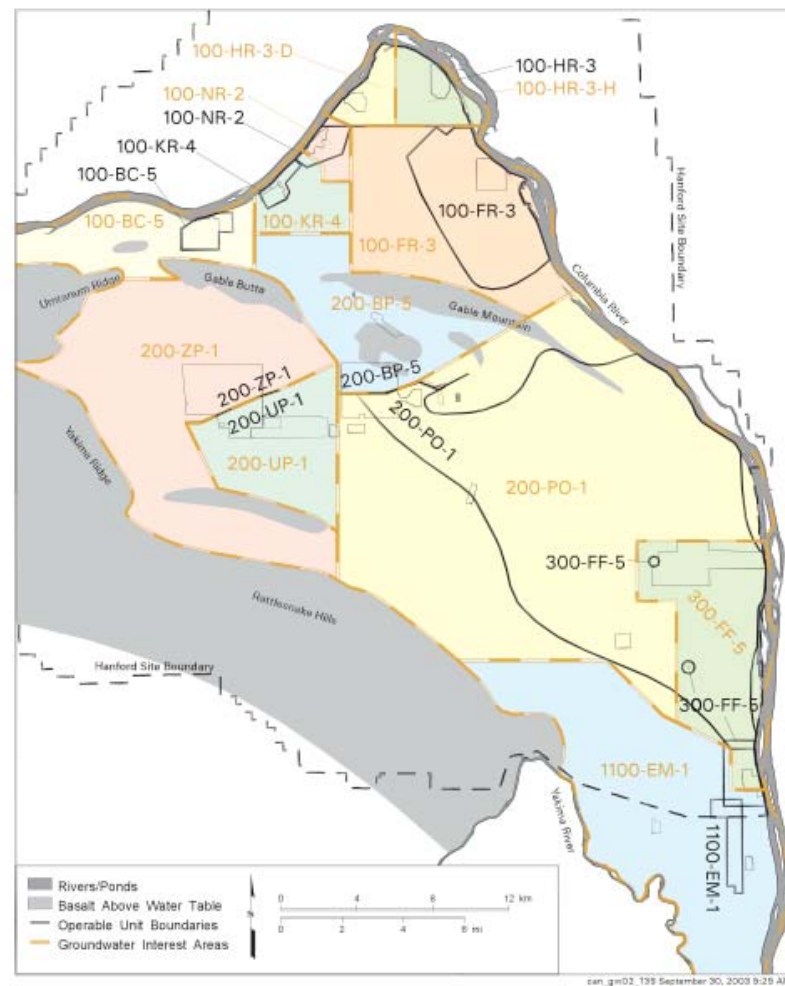


Figure 2.1-1. Groundwater Operable Units and Groundwater Interest Areas on the Hanford Site

Key Temporal Components

- Temporal variograms
 - Optimizes by determining sampling frequency associated with no average inter-event correlation
- Iterative fitting
 - Optimizes frequency at individual wells
 - Drops data until trends cannot be reconstructed
- Trend maps
 - By-product of iterative fitting
 - Provides spatial overview of site trends

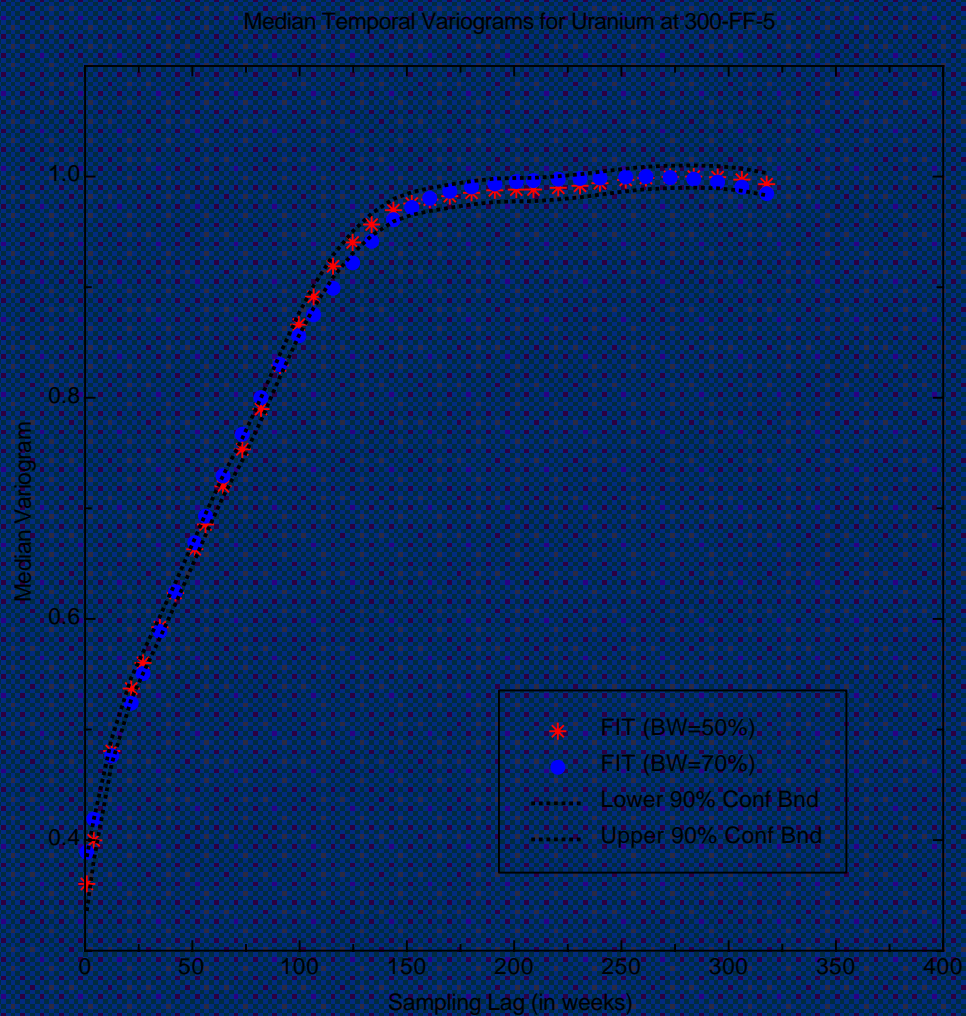
Temporal Variogram

- Useful with
 - Irregularly sampled data
 - Fewer samples (≥ 2 per well)
- Limitations
 - Must exclude wells with high ND rates ($>70\%$)
 - Averages correlation across wells
 - Complex trends, seasonal effects may impact overall performance
- Provides common sampling frequency for entire set of wells

Variogram Nuts & Bolts

- All possible pairs of squared differences formed at each well
 - Pairs pooled across wells
 - Differences unit-scaled to adjust for wells with much higher concentrations
- Local quadratic regression used to ‘smooth’ scatter cloud of differences
 - Confidence bands also computed
- Variogram range estimates point of no temporal correlation

Uranium Variogram



Iterative Fitting

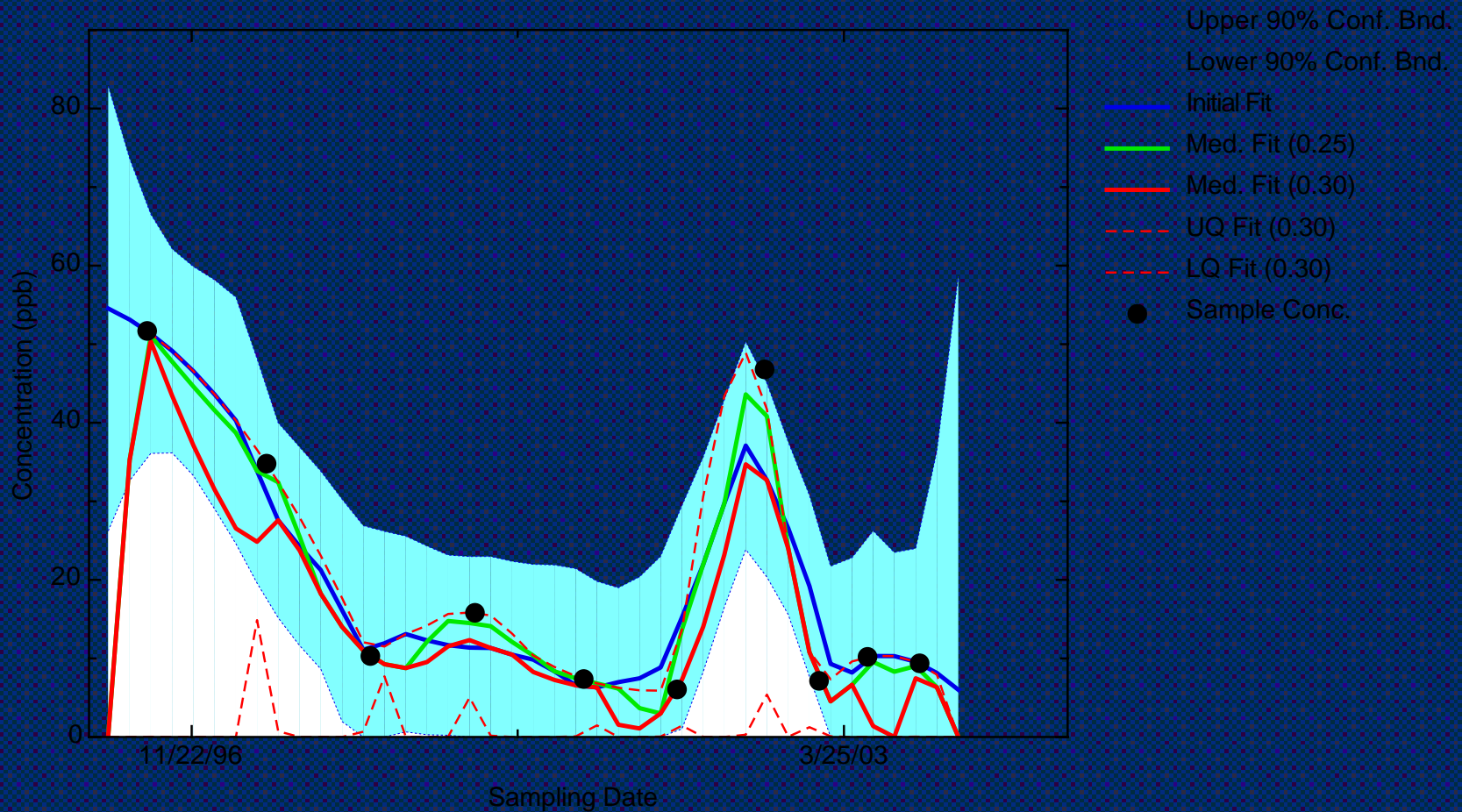
- Unique trend fit at each well
 - Confidence bands too
- Data removed until new trends fall outside confidence bands
- Optimized sampling interval computed from average remaining inter-event time
 - Median value across set of wells used to set common frequency

Data Requirements

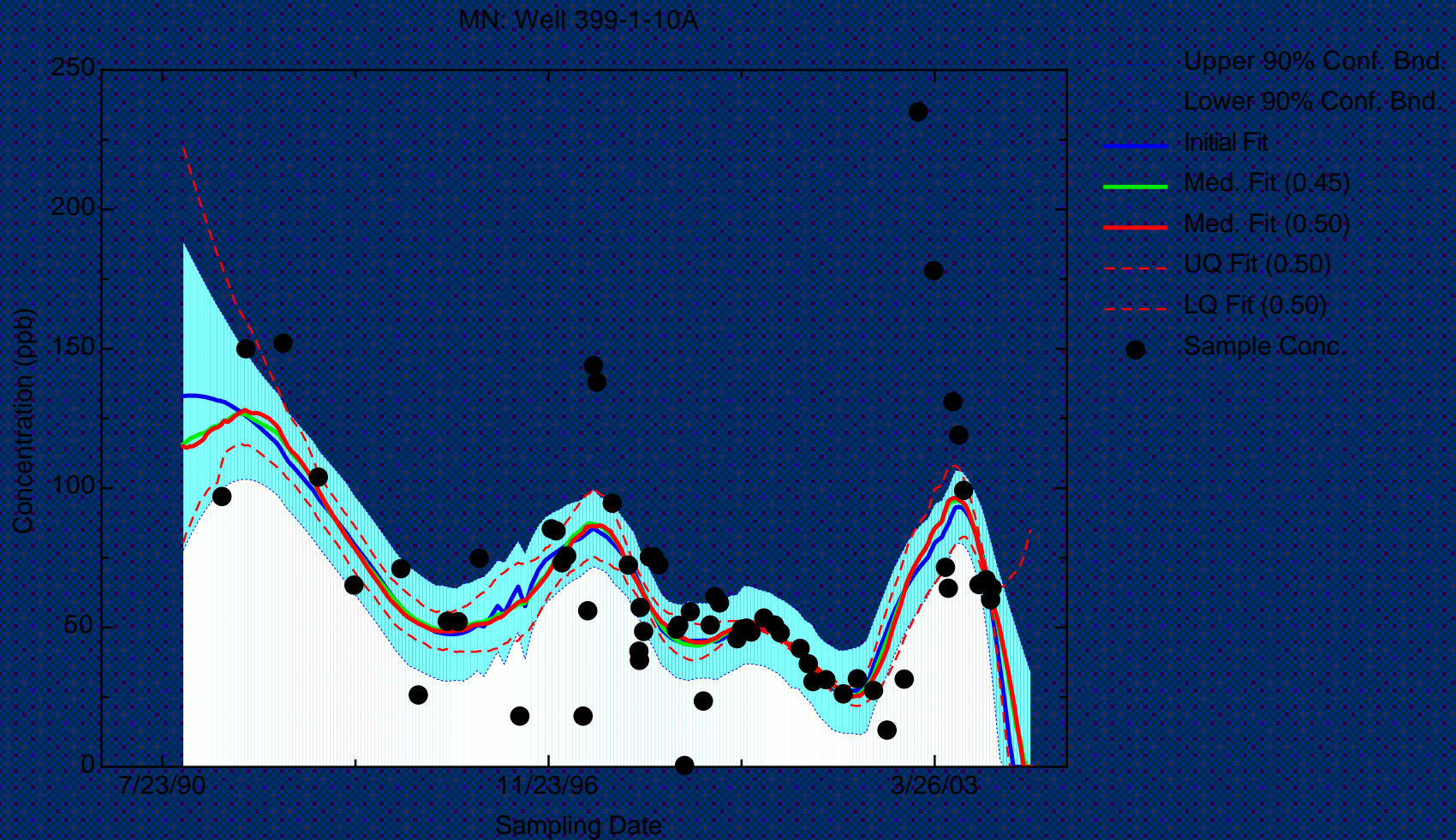
- Minimum of 8-10 sample events per well
- Must have some detects
 - GTS weeds out wells with no variation
 - Extreme outliers, data gaps are screened
- Seasonal trends no problem
 - GTS fits complex temporal patterns
 - Seasonal patterns should be evident in time series plots

Uranium Fitting Example 1

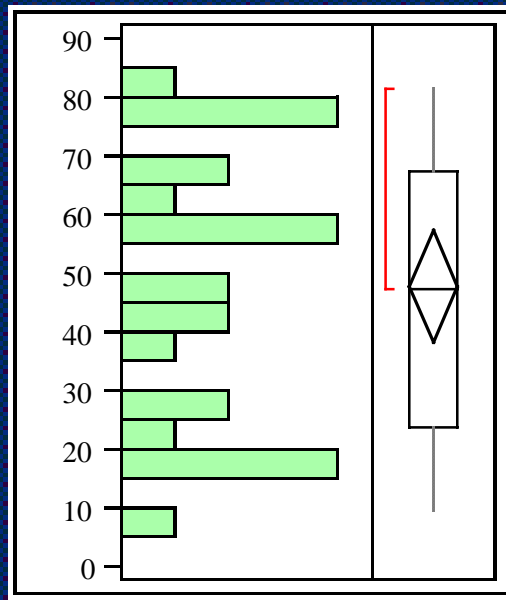
MN: Well 399-1-2



Uranium Fitting Example 2



Iterative Fitting Summary



| | |
|---------|--------|
| N Wells | 25 |
| LQ | 24 wks |
| Median | 47 wks |
| UQ | 67 wks |

Trend Mapping

- Post-plot of iterative fitting slopes
 - Historical (average) or recent trends plotted by GTS
 - Slopes ranked by relative magnitude, statistical confidence
- Indicates what areas of site are rising or falling

Post-Plot of Historical Median Trends for Uranium

The plot displays Northing (m) on the Y-axis (ranging from $1.1 \cdot 10^5$ to $1.2 \cdot 10^5$) versus Easting (m) on the X-axis (ranging from $5.932 \cdot 10^5$ to $5.944 \cdot 10^5$). The data points are categorized by trend:

- Downward/Flat (Cyan circles)
- Surely Downward (Blue circles)
- Upward (Magenta squares)
- Surely Upward (Orange squares)
- Surely Flat (Red squares)

Uranium Recent Trend Map

